

# Inversion symmetry breaking and criticality in free fermionic lattices

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We describe the connection between inversion symmetry breaking and criticality in free fermionic lattice models. It is shown that for translation-invariant spinless fermions, the breaking of this symmetry in the ground state implies criticality, i.e., the existence of long-range correlations and the vanishing of the spectral gap; while for models with spin, only the asymmetry of the spin-averaged covariance matrix implies a similar conclusion. Our results are proved by introducing invariants under global translation-invariant free fermion quenches. Using this result, we identify a set of models where the generalized Hartree-Fock approximation must break down.

## I. INTRODUCTION

Symmetries play a prominent role in the characterization of many-body systems. A very timely topic in this respect is, for example, the theory of topological insulators and superconductors [1]. These phases of matter are modelled on free fermion lattices, gapped and possess a topological invariant that does not change its value if one adiabatically changes the system by local perturbations that preserve certain symmetries and do not close the gap. In this paper, we describe a dual result: we introduce quantities that are invariant under sudden global (translation-invariant) quenches, and whose non-zero expectation values imply criticality.

The introduced invariants are connected to the inversion symmetry breaking of the ground state. In our setup the free fermion Hamiltonians explicitly break this symmetry, and we show that they can only be gapped if the expectation values of these invariants vanishes in the ground state.

Inversion symmetry breaking lattice models appear in the realm of many physical scenarios, e.g., in non-equilibrium states [2, 3], in the case of Dzyaloshinskii-Moriya interactions [4–7], or in directed quantum transport [8]. In a previous work, we noticed that when the covariance matrix of a translation-invariant spinless free-fermion chain breaks reflection symmetry (which is identical to inversion in one dimension), it is necessarily gapless [9]. This finding lead us to study whether a similar statement holds with spin degrees of freedom and/or in higher-dimensions. Using the structure of the general Hamiltonian describing translation-invariant  $d$  dimensional spinful quasifree models, we introduce a set of invariants connected to inversion symmetry breaking that can be used to signal criticality. Concerning topological insulators and superconductors, this result implies that the models are either interacting or inversion symmetry breaking happens at the quantum critical point [10–13].

When the expectation values of the mentioned invari-

ants do not vanish in a translation-invariant quasifree state, the area law for the entanglement entropy is logarithmically violated. An immediate consequence of this is the breakdown of the generalized Hartree-Fock method and band model approximations for certain interacting gapped models with inversion symmetry breaking.

The paper is structured as follows. In Section II we introduce quasifree fermion models, and provide their ground-state two-point function in full generality. The main result is stated and proved in Section III, after an example of a gapped pairing model, which shows that the naive generalization of the spinless invariants does not work. Finally, the insufficiencies of generalized Hartree-Fock approximation is explained.

## II. REFLECTION SYMMETRY IN FREE FERMION HAMILTONIANS

### A. The model

We consider a  $d$  dimensional cubic lattice of fermions with arbitrary spin. The fermion operator  $b_n^j$  is the annihilation operator at the lattice point denoted by  $n \equiv (n_1, n_2, \dots, n_d)$ , where  $n_i \in \{1, 2, \dots, N_i\}$ , and the spin index  $j \in \{1, 2, \dots, s\}$ , the creation operators  $b_n^{j\dagger}$  have analogous notation. The most general quadratic combination of these fermion operators yielding a Hermitian operator on the Fock space reads

$$H = \sum_{j,l=1}^s \sum_{m,n=1}^N A_{mn}^{jl} b_m^{j\dagger} b_n^l + \frac{1}{2} \left( B_{mn}^{jl} b_m^{j\dagger} b_n^{l\dagger} - \bar{B}_{mn}^{jl} b_m^j b_n^l \right), \quad (1)$$

where summation of  $m$  and  $n$  is over the sites  $N$  of the lattice (e.g., for a square lattice in dimension two, the multi-index  $m \equiv (m_1, m_2)$  labels all  $N \equiv N_1 N_2$  sites in the natural way). We assume periodic boundary conditions. Without loss of generality one can impose that  $B_{mn}^{jl} = -B_{nm}^{jl}$ , and the constraint  $H^\dagger = H$  is equivalent to  $A_{mn}^{jl} = \bar{A}_{nm}^{lj}$ .

We shall often write the  $Ns$  dimensional vector  $b$  ( $b^\dagger$ ) without indices, whose components are  $b_m^j$  ( $b_m^{j\dagger}$ , respectively). It is customary to write the above Hamiltonian

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as

$$H = \frac{1}{2} \begin{pmatrix} b^\dagger & b \end{pmatrix} \begin{pmatrix} A & B \\ -B^\dagger & -A^T \end{pmatrix} \begin{pmatrix} b \\ b^\dagger \end{pmatrix}, \quad (2)$$

where the big matrix of size  $2sN \times 2sN$  is called the Bogoliubov–de Gennes (BdG) Hamiltonian.

Translation invariance implies that all the coefficient matrices are circulant:  $X_{m+p,n+p}^{jl} = X_{m,n}^{jl}$  for any translation  $p \equiv (p_1, p_2, \dots, p_d)$  (addition, subtraction and scalar multiplication between multi-indices are naturally meant componentwise). The periodic boundary condition is taken into account through the definitions  $b_n^j = b_{n+\underline{N}}^j$ , with  $\underline{N} \equiv (N_1, N_2, \dots, N_d)$ .

### B. Two-point function of the ground state

Let us fix our conventions used in the calculation. The Fourier of the one-particle annihilation operators and its inverse read (we use the variable  $k$  or  $k'$  exclusively for the Fourier transform in what follows)

$$b_k^j = \frac{1}{\sqrt{N}} \sum_n \exp\left(-\frac{2\pi i n k}{N}\right) b_n^j, \quad (3)$$

$$b_n^j = \frac{1}{\sqrt{N}} \sum_k \exp\left(\frac{2\pi i n k}{N}\right) b_k^j, \quad (4)$$

where  $N \equiv \prod_i^d N_i$ ,  $k \equiv (k_1, k_2, \dots, k_d)$ ,  $nk \equiv \sum_i^d n_i k_i$  and there are  $d$  summations over  $n_i$  or  $k_i$ ,  $i = 1, 2, \dots, d$ , that is, the  $i$ -th component of  $n$  and  $k$  run in from 1 to  $N_i$ . The transform of the one-particle creation operators are to be computed by means of taking the adjoint of the above formulae.

For circulant matrices we define the Fourier transform as

$$X_k^\xi = \sum_n \exp\left(-\frac{2\pi i n k}{N}\right) X_{n\mathbf{0}}^\xi, \quad (5)$$

$$X_{n\mathbf{0}}^\xi = \frac{1}{N} \sum_k \exp\left(\frac{2\pi i n k}{N}\right) X_k^\xi, \quad (6)$$

where  $\xi$  stands for the pair of spin indices ( $\mathbf{0}$  is the  $d$  dimensional zero vector). Summation conventions are identical to the above.

Using these definitions, the Hamiltonian (1) or (2) can be written as

$$H = \frac{1}{2} \sum_k \begin{pmatrix} b_k^\dagger & b_{-k} \end{pmatrix} \begin{pmatrix} A_k & B_k \\ B_k^\dagger & -A_{-k}^T \end{pmatrix} \begin{pmatrix} b_k \\ b_{-k}^\dagger \end{pmatrix}, \quad (7)$$

where the  $2s \times 2s$  big matrix is denoted by  $\mathcal{H}_k$ , and is called the Bogoliubov-de Gennes (BdG) Hamiltonian. The hermiticity constraint imply

$$A_k^\dagger = A_k, \quad B_{-k} = -B_k^T, \quad (8)$$

and in particular,  $A_k^{jj} \in \mathbb{R}$  and  $B_{-k}^{jj} = -B_k^{jj}$ .

To bring this Hamiltonian into a diagonal form

$$H = \sum_{j=1}^s \sum_k \Lambda_k^j c_k^{j\dagger} c_k^j, \quad (\Lambda_k^j \in \mathbb{R}),$$

one performs a Bogoliubov transformation [17]

$$c_k^j = \sum_{l=1}^s \left( \alpha_k^{jl} b_k^l + \beta_k^{jl} b_{-k}^{l\dagger} \right), \quad \alpha_k^{jl}, \beta_k^{jl} \in \mathbb{C}, \quad (9)$$

where the coefficients  $\alpha_k^{jl}, \beta_k^{jl}$  have to satisfy for each  $j, j' \in \{1, 2, \dots, s\}$

$$\sum_{l=1}^s \left( \alpha_k^{jl} \beta_{-k}^{j'l} + \beta_k^{jl} \alpha_{-k}^{j'l} \right) = 0, \quad (10)$$

$$\sum_{l=1}^s \left( \alpha_k^{jl} \bar{\alpha}_k^{j'l} + \beta_k^{jl} \bar{\beta}_k^{j'l} \right) = \delta_{jj'}, \quad (11)$$

so that the canonical anticommutation relations  $\{c_k^j, c_{k'}^{j'\dagger}\} = \delta_{jj'} \delta_{kk'}$ ,  $\{c_k^j, c_{k'}^j\} = 0$  are satisfied. The consistency conditions for the commutator

$$[c_k^j(b), H(b)] = \Lambda_k^j c_k^j(b)$$

yield the eigenvalue equations[18]

$$\mathcal{H}_k v_k^j = \Lambda_k^j v_k^j \quad (12)$$

with  $v_k^j \equiv (\bar{\alpha}_k^{j1}, \bar{\alpha}_k^{j2}, \dots, \bar{\alpha}_k^{js}, \bar{\beta}_k^{j1}, \bar{\beta}_k^{j2}, \dots, \bar{\beta}_k^{js})$ . Let us use the notations  $\Psi_k \equiv (b_k, b_{-k}^\dagger)$  and  $\tilde{\Psi}_k \equiv (c_k, c_{-k}^\dagger)$  to write  $2H = \Psi_k^\dagger \mathcal{H}_k \Psi_k = \tilde{\Psi}_k^\dagger \mathcal{H}_k^d \tilde{\Psi}_k$  with  $\mathcal{H}_k^d$  diagonal matrix. The generic BdG Hamiltonian satisfies

$$\sigma_x^{ph} \mathcal{H}_k \sigma_x^{ph} = -\bar{\mathcal{H}}_{-k} \quad (13)$$

with  $\sigma_x^{ph}$  being the first Pauli matrix acting in the “particle-hole” space (that is, the indicated splitting of the  $2s$  by  $2s$  matrix into  $s$  by  $s$  blocks). The property (13) is sometimes called particle-hole symmetry. Note, that this is *always* present in translational invariant quasifree fermion systems. As a consequence, the form of the diagonal Hamiltonian reads  $\mathcal{H}_k^d = \text{diag}(\Lambda_k^1, \Lambda_k^2, \dots, \Lambda_k^s, -\Lambda_{-k}^1, -\Lambda_{-k}^2, \dots, -\Lambda_{-k}^s)$ . The unitary defined by  $\Psi_k = U \tilde{\Psi}_k$  can be read off from the inverse of (9)

$$b_k^j = \sum_{l=1}^s \left( \bar{\alpha}_k^{lj} c_k^l + \beta_{-k}^{lj} c_{-k}^{l\dagger} \right), \quad (14)$$

it reads

$$U = \begin{pmatrix} \alpha_k^\dagger & \beta_{-k}^T \\ \beta_k^\dagger & \alpha_{-k}^T \end{pmatrix} \quad (15)$$

and the eigenvectors of  $\mathcal{H}_k$  are its columns by definitions.

In the ground state, the two-point functions of the new Fermi operators read

$$\langle c_k^{j\dagger} c_{k'}^{j'} \rangle = \frac{1}{2} \left( -\frac{\Lambda_k^j}{|\Lambda_k^j|} + 1 \right) \delta_{j,j'} \delta_{k,k'}, \quad (16)$$

$$\langle c_k^{j\dagger} c_{k'}^{j'\dagger} \rangle = \langle c_k^{j\dagger} c_{k'}^{j'\dagger} \rangle = 0. \quad (17)$$

Using these we can express those of the original ones using (14) (summation over the Fourier  $k$  and the spin index  $l$ )

$$\begin{aligned} \langle b_m^j b_n^{j'} \rangle &= \frac{1}{2N} \sum_{k,l} \exp \frac{2\pi i k(m-n)}{N} (bb)_k^{l,j,j'} \\ \langle b_m^{j\dagger} b_n^{j'} \rangle &= \frac{1}{2N} \sum_{k,l} \exp \frac{2\pi i k(m-n)}{N} (b^\dagger b)_k^{l,j,j'} \end{aligned}$$

with the kernels

$$\begin{aligned} (bb)_k^{l,j,j'} &\equiv \bar{\alpha}_k^{lj} \beta_k^{lj'} \left( \frac{\Lambda_k^l}{|\Lambda_k^l|} + 1 \right) + \beta_{-k}^{lj} \bar{\alpha}_{-k}^{lj'} \left( -\frac{\Lambda_{-k}^l}{|\Lambda_{-k}^l|} + 1 \right) \\ (b^\dagger b)_k^{l,j,j'} &\equiv \alpha_{-k}^{lj} \bar{\alpha}_{-k}^{lj'} \left( -\frac{\Lambda_{-k}^l}{|\Lambda_{-k}^l|} + 1 \right) + \bar{\beta}_k^{lj} \beta_k^{lj'} \left( \frac{\Lambda_k^l}{|\Lambda_k^l|} + 1 \right) \end{aligned}$$

Now, let us introduce the following notations

$$M_k^l = \frac{1}{2} \left( \frac{\Lambda_k^l}{|\Lambda_k^l|} - \frac{\Lambda_{-k}^l}{|\Lambda_{-k}^l|} \right), \quad P_k^l = \frac{1}{2} \left( \frac{\Lambda_k^l}{|\Lambda_k^l|} + \frac{\Lambda_{-k}^l}{|\Lambda_{-k}^l|} \right),$$

$$(S_k^{l\pm})_{jj'} = \bar{\alpha}_k^{lj} \beta_k^{lj'} \pm \beta_{-k}^{lj} \bar{\alpha}_{-k}^{lj'}, \quad (Z_k^{l\pm})_{jj'} = \bar{\alpha}_k^{lj} \alpha_k^{lj'} \pm \beta_{-k}^{lj} \bar{\beta}_{-k}^{lj'},$$

in terms of which the kernels defined above can be conveniently written as

$$(bb)_k^{l,j,j'} = (M_k^l + 1)(S_k^{l+})_{jj'} + P_k^l(S_k^{l-})_{jj'} \quad (18)$$

$$(b^\dagger b)_k^{l,j,j'} = (M_k^l + 1)(\overline{Z_{-k}^{l+}})_{jj'} - P_k^l(\overline{Z_{-k}^{l-}})_{jj'} \quad (19)$$

Before analysing these results from the point of view of inversion symmetry breaking, we write down the following useful set of identities:

$$\begin{aligned} \sum_{l=1}^s S_k^{l+} &= \mathbf{0}, \\ \sum_{l=1}^s (Z_k^{l+})_{jj'} &= \delta_{jj'}. \end{aligned} \quad (20)$$

They are the components of the matrix equation  $UU^\dagger = \mathbb{1}$  with  $U$  being the unitary defined by (15) (c.f., the components of the equation  $U^\dagger U = \mathbb{1}$  are equivalent to (10) and (11)).

### C. (Extended) inversion symmetry

The inversion symmetry transformation whose breaking is related to criticality is given by the transformation

$$b_m^j \mapsto i b_{-m}^j$$

implying  $A_{mn}^{jl} \mapsto \bar{A}_{mn}^{lj}$  and no change in the pairing coefficients  $B_{mn}^{jl}$ . Or using the notation  $A_{mn}$  for the  $s \times s$  matrix, whose entries are given by  $(A_{mn})_{jl} = A_{mn}^{jl}$  we can express the transformation as  $A_{mn} \mapsto A_{mn}^\dagger$ .

In case the model is spinless the formula from [9] relating the one-particle spectrum to the coefficients of the BdG Hamiltonian

$$\Lambda_k = \frac{A_k - A_{-k} + \sqrt{(A_k + A_{-k})^2 + 4B_k \bar{B}_k}}{2}, \quad (21)$$

applies (with  $k$  standing for the coordinate of the  $d$  dimensional momentum torus). In other words, since  $A_k - A_{-k} = \Lambda_k - \Lambda_{-k}$  and  $A_k - A_{-k} \neq 0$  means broken inversion symmetry, all we have to investigate is the dependence on the  $k$ -antisymmetric part of the one-particle spectrum.

In the mentioned previous work [9], the starting point was a quasifree spin chain, which by definition can be transformed by Jordan-Wigner transformation to a fermion chain. There, studying inversion symmetry breaking we arrived at the above conclusion and investigated when the ground state is sensitive to  $(\Lambda_k - \Lambda_{-k}) \neq 0$  [19]. We have found that only the imaginary part of the two-point functions  $\langle b_j^\dagger b_l \rangle$  depend on this quantity and that dependence appears via the combination  $M_k \sim (\Lambda_k/|\Lambda_k| - \Lambda_{-k}/|\Lambda_{-k}|)$ . If there is a momentum  $k_0$  with  $M_{k_0} \neq 0$ , this implies that  $\Lambda_{k_1} = 0$  at some momentum  $k_1$ . Consequently, the gap disappears whenever  $\text{Im}\langle b_j^\dagger b_l \rangle \neq 0$  (and the corresponding spin-chain ground state breaks inversion symmetry).

For the general quasifree fermion lattice we cannot express  $\Lambda_k^j$  explicitly in terms of the coefficients of the Hamiltonian (the solution of the characteristic equation of the  $2s \times 2s$  BdG matrix). But we can investigate if the non-vanishing of the quantity  $\text{Im}\langle b_m^{j\dagger} b_n^l \rangle$  or a suitably modified version of it signals inversion symmetry breaking and if it leads to criticality.

## III. THE MAIN RESULT

In higher dimensional and spinful quasifree fermionic lattices the non-vanishing of  $\text{Im}\langle b_m^{j\dagger} b_n^j \rangle$  [20] does *not* imply criticality: it is clearly demonstrated by the following simple model. Consider consider the following nearest-

neighbor spin- $\frac{1}{2}$  Hamiltonian given by

$$H = \frac{1}{2} \sum_m \left[ (p-1)(b_m^{\dagger\dagger} b_m^{\dagger} + b_m^{\dagger\dagger} b_m^{\dagger}) + \right. \\ \left. i \frac{p+1}{2} (-b_m^{\dagger\dagger} b_{m+1}^{\dagger} + b_{m+1}^{\dagger\dagger} b_m^{\dagger} + b_m^{\dagger\dagger} b_{m+1}^{\dagger} - b_{m+1}^{\dagger\dagger} b_m^{\dagger}) \right. \\ \left. - \frac{p+1}{2} (b_m^{\dagger\dagger} b_{m+1}^{\dagger} + b_{m+1}^{\dagger\dagger} b_m^{\dagger} + b_m^{\dagger\dagger} b_{m+1}^{\dagger} + b_{m+1}^{\dagger\dagger} b_m^{\dagger}) \right]$$

We assume that the parameter  $p > 0$ . In the momentum space (with the abbreviation  $\tilde{k} = 2\pi k/N$ ) it has the form

$$H = \sum_k \frac{p+1}{2} \sin \tilde{k} (b_k^{\dagger\dagger} b_k^{\dagger} - b_k^{\dagger\dagger} b_k^{\dagger}) + \frac{p-1}{2} (b_k^{\dagger\dagger} b_k^{\dagger} + b_k^{\dagger\dagger} b_k^{\dagger}) \\ - \frac{p+1}{2} \cos \tilde{k} (b_k^{\dagger\dagger} b_k^{\dagger} + b_k^{\dagger\dagger} b_k^{\dagger}) .$$

The diagonal form  $H = \sum_k (-c_k^{\dagger\dagger} c_k^{\dagger} + p c_k^{\dagger\dagger} c_k^{\dagger})$  is obtained by the transformation

$$b_k^{\dagger} = \frac{1}{\sqrt{2}} \left( (\cos \tilde{k}/2 - \sin \tilde{k}/2) c_k^{\dagger} + (\cos \tilde{k}/2 + \sin \tilde{k}/2) c_k^{\dagger} \right) \\ b_k^{\dagger} = \frac{1}{\sqrt{2}} \left( (\cos \tilde{k}/2 + \sin \tilde{k}/2) c_k^{\dagger} - (\cos \tilde{k}/2 - \sin \tilde{k}/2) c_k^{\dagger} \right) ,$$

Now we can compute arbitrary two-point functions. In particular, we get

$$\langle b_m^{\dagger\dagger} b_{m+1}^{\dagger} \rangle = -\frac{i}{4} \quad \langle b_m^{\dagger\dagger} b_{m+1}^{\dagger} \rangle = \frac{i}{4} ,$$

showing that these quantities need not be real, although the model is gapped.

However, we found the proper generalization of the spinless one-dimensional result:

**Main result.** *Consider the ground state of a model given by the Hamiltonian (1), and let  $U$  be a unitary implementing an arbitrary translation-invariant Bogoliubov transformation. Then the following hold: (i)*

$$Im(\sum_{j=1}^s \langle b_m^j \dagger b_n^j \rangle) = Im(\sum_{j=1}^s \langle U b_m^j \dagger b_n^j U^{\dagger} \rangle) , \quad (22)$$

*i.e., the lhs. of (22) is  $U$ -invariant; (ii) if*

$$Im(\sum_{j=1}^s \langle b_m^j \dagger b_n^j \rangle) \neq 0$$

*for certain  $m$  and  $n$ , then the model is gapless.*

We will prove point (ii) of the proposition in the next subsection using directly the parameters of the diagonalization in Sec. II. Later in Sec. III.B we present a more abstract treatment, sketching a proof of (i) and through that an alternative simple proof of (ii).

## A. Direct parametrization method

To prove the proposition, we notice from the form of Eq. (19) that if  $M_k^l \equiv 0$  for all spin components  $l$ , then, without loss of generality we can assume that  $P_k^l \equiv 1$ . [21] We first write – using the identities (20) – the Fourier kernel of the two-point function (19) as

$$\sum_{l=1}^s (b^{\dagger} b)_k^{l,j,j} = 1 - \sum_{l=1}^s \overline{(Z_{-k}^{l-})_{jj}} = 1 + \sum_{l=1}^s (-|\alpha_{-k}^{lj}|^2 + |\beta_k^{lj}|^2) \\ = 1 - \sum_{l=1}^s (|\alpha_{-k}^{lj}|^2 + |\beta_k^{lj}|^2) + 2 \sum_l |\beta_k^{lj}|^2 \\ = 2 \sum_{l=1}^s |\beta_k^{lj}|^2 ,$$

where in the last equality we used (20) again. Now we need the summed version of two equation (11) and (20) to arrive at

$$\sum_{l,j=1}^s (|\alpha_k^{jl}|^2 + |\beta_k^{jl}|^2) = s = \sum_{l,j=1}^s (|\alpha_k^{jl}|^2 + |\beta_{-k}^{jl}|^2) .$$

This shows that  $\sum_{l,j} |\beta_k^{lj}|^2 = \sum_{l,j} |\beta_{-k}^{lj}|^2$ , which implies that the summed Fourier kernel  $\sum_{l,j} (b^{\dagger} b)_k^{l,j,j}$  is also symmetric in  $k$ . But it is also real, so the quantity  $\sum_j \langle b_m^j \dagger b_n^j \rangle$  is also real.

This means that if  $Im(\sum_j \langle b_m^j \dagger b_n^j \rangle) \neq 0$ , then at least for one  $j$  and  $k_0$  we have  $M_{k_0}^j = \frac{1}{2} (\Lambda_{k_0}^j / |\Lambda_{k_0}^j| - \Lambda_{-k_0}^j / |\Lambda_{-k_0}^j|) \neq 0$ , which, in turn, implies the absence of the gap as explained in the beginning of the section for the spinless case [22].

## B. Method of commuting invariants

We start by introducing a general Bogoliubov transformation, which is a basis change in the space of creation and annihilation operators

$$b_m^j \mapsto \mathcal{U} b_m^j \mathcal{U}^{\dagger}$$

which keep the canonical anticommutation relations invariant. Now we can turn to the proof, which is based on a result from [15] that the expression

$$C_n \equiv \frac{i}{2} \sum_{m,j} (b_{n+m}^{j\dagger} b_m^j - b_m^{j\dagger} b_{m+n}^j)$$

commutes with any quasifree Hamiltonian of the form (1). Writing down the expectation value in the ground state of a translation invariant Hamiltonian, the summation over  $m$  is over identical terms and we have

$$\langle C_n \rangle = N \langle Im \sum_j b_{n+m}^{j\dagger} b_m^j \rangle$$

and since any translation invariant Bogoliubov transformation can be written as  $U = e^{iH}$  with  $H$  translation invariant quasifree Hamiltonian, the invariance property (22) follows.

This gives a rather simple way to check its relation to the absence of the spectral gap, namely, we can look at the diagonal basis. The summed two-point function in the diagonal basis reads

$$\sum_j \langle b_m^\dagger b_n^j \rangle = \frac{1}{2N} \sum_{k,j} \exp \frac{2\pi i k(m-n)}{N} \left( -\frac{\Lambda_{-k}^j}{|\Lambda_{-k}^j|} + 1 \right)$$

Its imaginary part is proportional to the k-antisymmetric part of the Fourier kernel:

$$\sum_j \frac{1}{2} \left( \frac{\Lambda_k^j}{|\Lambda_k^j|} - \frac{\Lambda_{-k}^j}{|\Lambda_{-k}^j|} \right) = \sum_j M_k^j,$$

which vanishes unless  $M_{k_0}^{j_0} \neq 0$  for a  $j_0$  and  $k_0$ , and this means the model is gapless as explained before.

### C. Consequences for mean-field approximations

Our result does not hold for interactive systems, but it does for any translation invariant quasifree one, which is possibly used in a mean-field approximation. Hence, in case we find that (22) is non-vanishing for some  $m, n$  in a gapped ground state of an interacting system, then the mean-field approximation based on the quasifree state with the matching covariance matrix will not converge. More precisely, as a consequence of our result, the entanglement entropy of the latter state necessarily violates the area law and it has algebraically decaying correlations as opposed to the area law satisfying gapped ground state with exponentially decaying correlations it is supposed to approximate. The approximation obviously cannot work.

An example is the Majumdar-Ghosh model [14], a nearest-neighbour and next-nearest-neighbour Heisenberg chain:

$$H = J \sum_j S_j \cdot S_{j+1} + \frac{J}{2} S_j \cdot S_{j+2}$$

where  $S_m \cdot S_n = \sigma_m^x \sigma_n^x + \sigma_m^y \sigma_n^y + \sigma_m^z \sigma_n^z$  in terms of Pauli matrices  $\sigma_p$  at site  $p$ . Its two ground states are known to be the singlets  $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$  between sites  $2j, 2j+1$  for all  $j$  those between sites or  $2j+1, 2j+2$ . The model can be rewritten in fermionic language via the Jordan-Wigner transformation (see e.g., [16]):

$$H = J \sum_{l=1}^L \left[ \left( \frac{1}{2} c_l^\dagger c_{l+1} + \frac{1}{4} c_l^\dagger c_{l+2} - \frac{1}{2} c_l^\dagger c_{l+1}^\dagger c_{l+1} c_{l+2} + h.c. \right) + \left( c_l^\dagger c_l - \frac{1}{2} \right) \left( c_{l+1}^\dagger c_{l+1} - \frac{1}{2} \right) + \frac{1}{2} \left( c_l^\dagger c_l - \frac{1}{2} \right) \left( c_{l+2}^\dagger c_{l+2} - \frac{1}{2} \right) \right] \quad (23)$$

and rewriting the ground states also in the fermionic language, one finds that  $\langle c_l^\dagger c_{l+1} \rangle = \langle c_{l+1}^\dagger c_l \rangle = 1/4$ .

Now, we can perform a transformation  $c_l \mapsto c_l e^{i\alpha}$  with a parameter  $\alpha$ , which multiplies the coefficients of the first three term in (23) by  $e^{i\alpha}$  and the second and third terms by  $e^{2i\alpha}$ . More importantly the two-point function after the transformation is  $\langle c_l^\dagger c_{l+1} \rangle = \langle c_{l+1}^\dagger c_l \rangle = 1/4 e^{i\alpha}$ . Now, the quasifree translation invariant model, which one would use to define the mean field (or generalised Hartree-Fock) approximation, with this property is gapless as we proved. Thus it has logarithmically diverging entropy and algebraically decaying correlations, it cannot approximate the ground state of the gapped Majumdar-Ghosh model [23].

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- [19] Let us note that due to the non-local nature of the Jordan-Wigner transformation, the reflection symmetry transformation in the spin chain is not identical to that in the fermion model.
- [20] The correlator between different spin components is easily excluded: suitable simple Bogoliubov transformation results in non-real expectation value in a gapped ground state of spinful quasifree model.
- [21] The signs of  $\Lambda_k^j$  and  $\Lambda_{-k}^j$  may be simultaneously negative, but the translation-invariant Bogoliubov transformation  $c_k^j \leftrightarrow c_{-k}^{j\dagger}$  on the diagonal BdG Hamiltonian changes the sign of  $P_k^j$ .
- [22] Note gaplessness follows here for the decoupled band  $j$ , and consequently for the whole model.
- [23] This is why no complex solution for  $\langle c_l^\dagger c_{l+1} \rangle$  was found by Verkholyak, Honecker and Brenig in [16] for the mean field equations.